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# The statistical description of model bias as a method to account for model structure errors

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## Summary of key findings

In this study, an existing statistical approach to account for model structure deficiencies is tested on a simulated batch experiment to identify parameters of a kinetic model for substrate degradation in biological wastewater treatment processes. A reported problem that model structure errors, on the one hand, can be hard to detect in realistic experimental settings while, on the other hand, have a tremendous impact on the design of biological environmental processes. Here, we investigate whether this dilemma can be solved with a statistical description of model discrepancies, the so-called model bias. Our results show how estimation errors resulting from model structural errors in biokinetic models can be accounted for by adding an autocorrelated error process, which leads to more realistic, albeit larger, prediction uncertainties than current approaches. In addition, the resulting parameter estimate intervals tend to be more reliable.

## Background and relevance

Accurate models are a prerequisite for effective model-based design, operation, and control of biological processes, including biological wastewater treatment processes. Environmental engineers today can rely on commercial software for model parameter identification and even model structure selection, thanks to ever-increasing computational power. Despite this ability, it is common to stick to a particular model structure, such as the Monod switching function to model substrate affinity, even when there is little evidence that this is in fact the best fitting structure. Ill-chosen model structures can remain undetected under realistic experiments and potentially lead to a failure in process design as shown earlier (Neumann & Gujer, 2008). Despite such consequences, choosing a particular model structure is still motivated by considering *(i)* that a given model structure can be easy to interpret, *(ii)* that finding an optimal model structure is still a complex problem, and *(iii)* that enumerating a large library of model structures does not guarantee optimality (Refsgaard et al., 2006). In light of these arguments, it is of interest whether one can use familiar model structures of personal choice while accounting for the systematic errors that may result from such a choice. Including a term describing model bias in the output error model allows to do this for predictive purposes (Reichert & Schuwirth, 2012). The resulting prediction intervals become more reliable (i.e. encompass a greater percentage of validation data) even when the deterministic part of the model is structurally different from the true process. In this collaborative line of work, we evaluate if this approach is also effective to account for such model structure errors when the model parameter estimates are of primary interest. This particular contribution focuses on the results obtained for parameter estimation.

## Results and discussion

*Simulation experiments.* A batch experiment is simulated by means of the following process model:

$$\frac{dS}{dt} = r_{\max} \cdot \left(1 - e^{-S/K_S}\right) \quad (1)$$

$$Y = S + E \quad (2)$$

with $S(t)$ the simulated substrate concentration (initial value: $S_0 = S(t=0) = 5\ g/m^3$), $E$ the vector of measurement errors (Gaussian with zero mean and standard deviation $\sigma_E = 0.1$ g/m$^3$), and $Y$ the vector of noisy measurements of the substrate. The above model corresponds to a process with Tessier

kinetics. The maximum reaction rate, $r_{max}$, and the affinity constant, $K_S$, were set at to be 1 g/m$^3$.h and 0.3 g/m$^3$ as in Neumann & Gujer (2008). A batch experiment of 8 hours is simulated with measurements every 1/100 h.

*Parameter identification.* The first model (model 1) is structurally equal to the model described above. The estimated parameters are the initial substrate concentration ($S_0$=$S(t=0)$), the maximum reaction rate ($r_{max}$), the substrate affinity constant ($K_S$), and the measurement standard deviation ($\sigma_E$). In this case, there is obviously no model structure error so that the results obtained for this model act as a reference. A second model (model 2) is similar to the above, except that the substrate affinity switching function is replaced with the more conventional Monod function:

$$\frac{dS}{dt} = r_{\max} \cdot \frac{S}{K_S + S} \tag{3}$$

In this case, model structure error is present and would be left unaccounted for in standard parameter estimation approaches.. For both the first and the second model, an uninformative flat prior is applied to all parameters. To account for model structure error, the bias description method proposed in Reichert & Schuwirth (2012) is applied. Practically, this means that the measurement equation (Eq. 2) is replaced with the following equations:

$$Y = S + B + E \tag{4}$$

$$B = N(0, \Sigma(\sigma_b, \tau)) \tag{5}$$

in which $B$ corresponds to the so called bias term which describes an auto-correlated noise process characterized by the parameters $\sigma_b$ (standard deviation) and $\tau$ (correlation length). This modification of the measurement model is implemented for both the Tessier and Monod models described above. Model 3 (Tessier kinetics with bias descriptor) allows evaluating what the effect of incorporating a bias term is when, in fact, it is not needed. Whereas for the Monod kinetics (model 4), the expected benefit of adding the bias description to a model with structural errors can be evaluated. For models 3 and 4, the set of phenomenological parameters are the same as above (models 1 and 2) in addition to the bias description parameters ($\sigma_b$, $\tau$). For the latter parameters, a weak exponential prior has been applied, reflecting our preference to favor small biases.

*Parameter densities.* Figures 1 and 2 show the probability densities for the identified parameters in the models. The parameter estimates for the Tessier models (left panels in Figure 1 and 2) exhibit limited bias and variance, as expected. Adding a bias term has a limited effect on the marginal distributions of the deterministic parameters. The situation is different for the Monod models. Without bias description (Figure 1, left), severe bias results, especially for the $K_S$ value. The slope of the growth rate function at zero substrate concentrations is defined by $K_S$ and is severely underestimated in this case. Adding the bias term improves its estimate; however, at the expense of increased uncertainty. In other words the bias description learns from the systematic mismatches observed during calibration and reacts by decreasing our confidence in the estimation of the parameters (Del Giudice et al., 2015).

*Discussion.* Our results clearly demonstrate that it is possible to account for systematic prediction errors due to an ill-specified model structure by means of augmenting the measurement error model with a stochastic bias term. Future work will focus on its applicability for improved process design.

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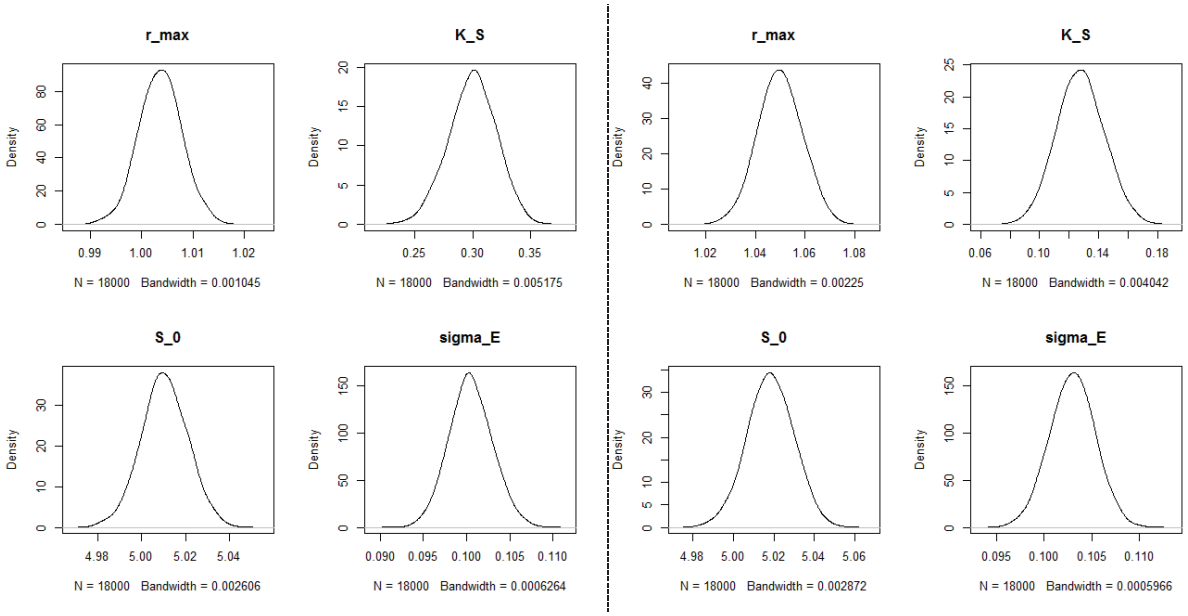


**Figure 1. Marginal posterior densities for models without bias term. Left: Tessier kinetics (model 1). Right: Monod kinetics (model 2).**

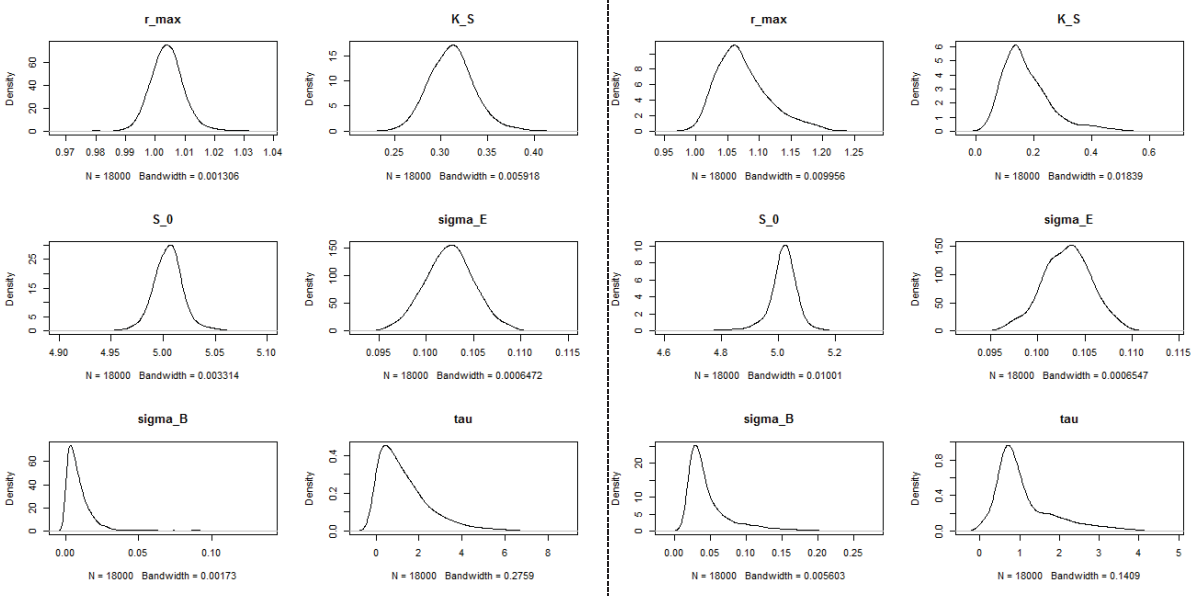


**Figure 2. Marginal posterior densities for models with bias term. Left: Tessier kinetics (model 3). Right: Monod kinetics (model 4).**